

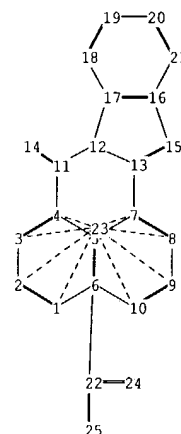
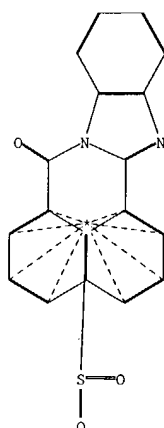
WEST Search History

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DATE: Sunday, March 21, 2004

<u>Hide?</u>	<u>Set Name</u>	<u>Query</u>	<u>Hit Count</u>
		<i>DB=USPT,EPAB,JPAB,DWPI,TDBD; PLUR=NO; OP=ADJ</i>	
<input type="checkbox"/>	L3	us-2949467-\$.did. or us-4024144-\$.did. or us-5470921-\$.did.	6
<input type="checkbox"/>	L2	us-6583284-\$.did.	2
<input type="checkbox"/>	L1	jp-51111237-\$.did. or jp-52072726-\$.did. or jp-58057463-\$.did.	6

END OF SEARCH HISTORY



chain nodes :

14 22 24 25

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 15 16 17 18 19 20 21

chain bonds :

11-14 22-24 22-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-13 8-9 9-10 11-12 12-13 12-17
13-15 15-16 16-17 16-21 17-18 18-19 19-20 20-21

exact/norm bonds :

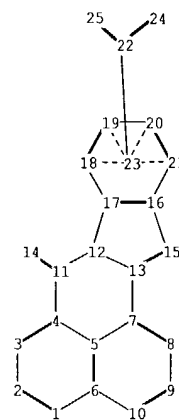
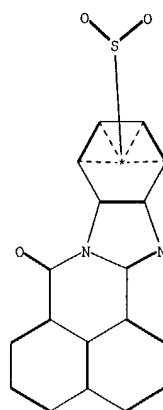
4-11 7-13 11-12 11-14 12-13 12-17 13-15 15-16 22-24 22-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:CLASS 23:CLASS 24:CLASS 25:CLASS



chain nodes :

14 22 24 25

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 15 16 17 18 19 20 21

chain bonds :

11-14 22-24 22-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 4-11 5-6 5-7 6-10 7-8 7-13 8-9 9-10 11-12 12-13 12-17
13-15 15-16 16-17 16-21 17-18 18-19 19-20 20-21

exact/norm bonds :

4-11 7-13 11-12 11-14 12-13 12-17 13-15 15-16 22-24 22-25

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-10 7-8 8-9 9-10 16-17 16-21 17-18 18-19
19-20 20-21

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
22:CLASS 23:CLASS 24:CLASS 25:CLASS

=> d his

(FILE 'HOME' ENTERED AT 19:32:35 ON 21 MAR 2004)

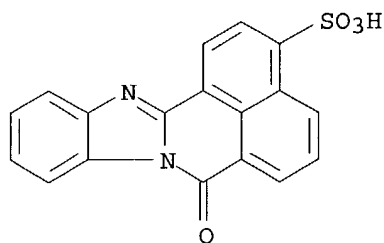
FILE 'REGISTRY' ENTERED AT 19:32:42 ON 21 MAR 2004

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L2	STRUCTURE UPLOADED
L3	19 S L1 OR L2
L4	STRUCTURE UPLOADED
L5	STRUCTURE UPLOADED
L6	4 S L4 OR L5
L7	112 S L4 OR L5 FUL

RN 41537-57-9 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-3-sulfonic acid, 7-oxo-, sodium
 salt (9CI) (CA INDEX NAME)
 MF C18 H10 N2 O4 S . Na
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
=====	=====	=====	=====	=====	=====
C3N2-C5N-C6- C6-C6	NCNC2-NC5-C6- C6-C6	5-6-6-6-6	C18N2	6841.6.3	1



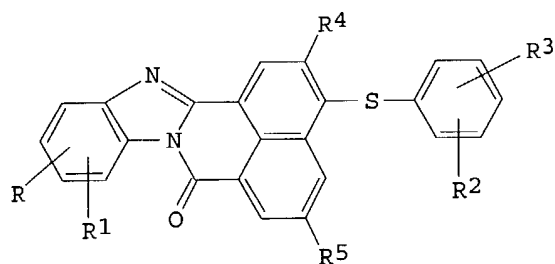
● Na

2 REFERENCES IN FILE CA (1907 TO DATE)
 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

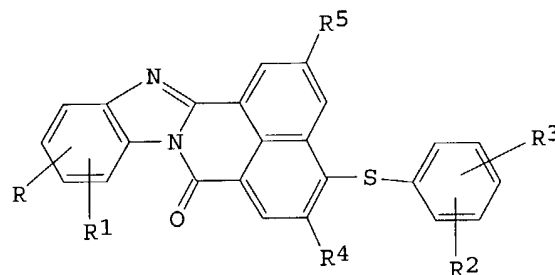
REFERENCE 1

AN 86:191337 CA
 TI 1,8-Naphthoylenebenzimidazole derivatives
 IN Shirosaki, Tsutomu
 PA Nippon Kayaku Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC C09B057-00
 CC 40-10 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
 Section cross-reference(s): 28
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	JP 51111237	A2	19761001	JP 1975-36069	19750327
PRAI	JP 1975-36069		19750327		
GI					



I



II

- AB I-II mixts. (R = H, Me, OMe, Bu, NO₂, Cl, CO₂H; R₁ = H, Me; R₂ = H, NH₂, Bu, Me, OMe; R₃ = H, Cl, Me, CO₂H; R₄ = H, Cl, Br, OH, OMe, OPr; R₅ = H, Cl, Br, OH, OMe, OPr, NO₂, SO₂NMe₂, SO₂NEt₂) useful as thioxanthene dye intermediates and as colorants for plastics and hydrophobic fibers were prepared For example, 1,2-benzenediamine [95-54-5] was stirred with 4-sulfonaphthalic anhydride Na salt [62635-64-7] in water at 98° for 12 h and then autoclaved with 2-aminobenzenethiol [137-07-5] in the presence of K₂CO₃ and Na₂SO₃·7H₂O at 150° for 10 h and at 170° for 12 h to give I-II mixture (all R's = H except R₂ = 2-NH₂); about 34 I-II mixts. were prepared
- ST phenylthionaphthoylenebenzimidazole deriv manuf; naphthoylenebenzimidazole phenylthio deriv
- IT Dyes
(intermediates, (phenylthio)naphthoylenebenzimidazole derivs.)
- IT 41537-57-9P 62602-99-7P
RL: PREP (Preparation)
(manufacture and reaction with aminobenzenethiol)
- IT 62599-17-1P 62599-18-2P 62599-40-0P 62599-41-1P
RL: PREP (Preparation)
(manufacture and reaction with aminomethylbenzenethiol)
- IT 5654-32-0P 5722-97-4P 53304-39-5P 53304-40-8P 62598-76-9P
62598-77-0P 62598-78-1P 62598-79-2P 62598-80-5P 62598-81-6P
62598-82-7P 62598-83-8P 62598-84-9P 62598-85-0P 62598-86-1P
62598-87-2P 62598-88-3P 62598-89-4P 62598-90-7P 62598-91-8P
62598-92-9P 62598-93-0P 62598-94-1P 62598-95-2P 62598-96-3P
62598-97-4P 62598-98-5P 62598-99-6P 62599-00-2P 62599-01-3P
62599-02-4P 62599-03-5P 62599-04-6P 62599-05-7P 62599-06-8P
62599-07-9P 62599-08-0P 62599-09-1P 62599-10-4P 62599-11-5P
62599-12-6P 62599-13-7P 62599-14-8P 62599-15-9P 62599-16-0P
62599-19-3P 62599-20-6P 62599-21-7P 62599-22-8P 62599-23-9P
62599-24-0P 62599-25-1P 62599-26-2P 62599-27-3P 62599-28-4P
62599-29-5P 62599-38-6P 62599-39-7P 62602-96-4P 62602-97-5P
62602-98-6P 62603-00-3P 62603-01-4P 62624-66-2P 62624-67-3P
62624-68-4P 62624-69-5P 62624-70-8P 62635-63-6P 62653-53-6P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)
- IT 62635-64-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzenediamine)
- IT 95-54-5, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with sulfonaphthalic anhydride sodium salt)
 IT 106-45-6 137-07-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with sulfonaphthoylenebenzimidazole)
 IT 2396-68-1 23451-96-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with sulfonaphthoylenebenzimidazole derivs.)

REFERENCE 2

AN 78:124591 CA
 TI Hydrazinoperinones
 IN Okada, Hiroshi; Kaneko, Masaharu; Kato, Yoshiaki
 PA Mitsubishi Chemical Industries Co., Ltd.
 SO Jpn. Kokai Tokkyo Koho, 5 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 NCL 16E6
 CC 28-10 (Heterocyclic Compounds (More Than One Hetero Atom))
 FAN.CNT 1

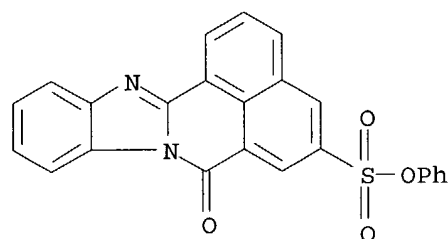
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 48013385	B4	19730220	JP 1971-42394	19710614
	JP 50036447		19750000	JP	

GI For diagram(s), see printed CA Issue.
 AB The title compds. (I where X = NHHN2), dye and pigment intermediates, were prepared E.g., 7.5 g I (X = SO3Na, Y = H) in H2O was refluxed 6 hr with 4 g N2H4.H2O to give 5 g I (X = NHHN2, Y = H). Similarly prepared were the following I (X = NHHN2) (Y given): x-Cl; x-NO2; x-OMe; x-Me. Also prepared were II and III.
 ST hydrazinoperinone dye intermediate; perinone hydrazino dye intermediate
 IT Dyes
 Pigments
 (intermediates for, hydrazinoperinones derivs. as)
 IT 41537-58-0P 41537-59-1P 41537-60-4P 41576-18-5P 41576-19-6P
 41576-20-9P 41576-21-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 41537-57-9
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction with hydrazine)

RN 58373-92-5 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-5-sulfonic acid, 10(or
 11)-ethoxy-7-oxo-, phenyl ester (9CI) (CA INDEX NAME)
 MF C26 H18 N2 O5 S
 CI IDS
 LC STN Files: CA, CAPLUS, IFICDB, IFIPAT, IFIUDB, USPATFULL

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
=====	=====	=====	=====	=====	=====
C6	C6	6	C6	46.150.18	1
C3N2-C5N-C6-	NCNC2-NC5-C6-	5-6-6-6-6	C18N2	6841.6.3	1
C6-C6	C6-C6				



D1-O-Et

1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 84:91652 CA
 TI Polycyclic dyes
 IN Groll, Manfred; Hederich, Volker; Bien, Hans S.
 PA Bayer A.-G., Fed. Rep. Ger.
 SO Ger. Offen., 38 pp.
 CODEN: GWXXBX
 DT Patent
 LA German
 IC C08K
 CC 40-6 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----	----	-----	-----	-----
PI	DE 2424542	A1	19751211	DE 1974-2424542	19740521
	GB 1451304	A	19760929	GB 1975-18965	19750506
	CH 613986	A	19791031	CH 1977-655	19750516
	JP 50161523	A2	19751227	JP 1975-58772	19750519
	US 4024144	A	19770517	US 1975-578770	19750519
	FR 2272152	A1	19751219	FR 1975-15846	19750521
	FR 2272152	B1	19790330		
PRAI	DE 1974-2424542		19740521		
GI	For diagram(s), see printed CA Issue.				
AB	Isomeric mixts. of polycyclic dyes (I R = H, iso-C8H17; X = o-phenylene,				

naphthylene; X1 = X, substituted 1,8-naphthylene or o-phenylene) and their brominated derivs. were prepared and used to dye polyester fibers fast yellow to red shades. Thus, a mixture of o-C6H4(NH2)2 [95-54-5] and 3-(phenoxy sulfonyl)naphthalic anhydride [58370-80-2] in HOAc was refluxed until the reaction was completed, the solution cooled, and II [58370-90-4] and its isomer [58370-91-5] were isolated. The other I were similarly prepared

ST phenyl polycyclic sulfonate dye; polyester fiber dye; isoquinoline sulfonate ester dye; perinone dye; phthaloperinone dye; naphthoylenebenzimidazole dye

IT Polyester fibers
 RL: USES (Uses)
 (dyes for, naphthoylenebenzimidazole and phthaloperinone sulfo derivs. as)

IT Dyes
 (naphthoylenebenzimidazole and phthaloperinone sulfo derivs., polyester fibers)

IT 14H-Benz[4,5]isoquino[2,1-a]perimidine-12-sulfonic acid, 14-oxo-, phenyl ester, bromo derivative
 14H-Benz[4,5]isoquino[2,1-a]perimidine-9-sulfonic acid, 14-oxo-, phenyl ester, bromo derivative
 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-2-sulfonic acid, 7-oxo-, phenyl ester, bromo derivative
 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-5-sulfonic acid, 7-oxo-, phenyl ester, bromo derivative
 RL: TEM (Technical or engineered material use); USES (Uses)
 (dye, for polyester fibers, preparation of)

IT 58370-86-8 58370-87-9 58370-88-0 58370-89-1 58370-90-4
 58370-91-5 58373-84-5 58373-85-6 58373-89-0 58373-90-3
 58373-91-4 58373-92-5 58374-12-2 58374-13-3 58676-84-9
 RL: TEM (Technical or engineered material use); USES (Uses)
 (dye, for polyester fibers, preparation of)

IT 58373-88-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction with phenol)

IT 1197-37-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with (phenoxy sulfonyl)naphthalic acid derivative)

IT 95-54-5, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with (phenoxy sulfonyl)naphthalic anhydride)

IT 479-27-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with (phenoxy sulfonyl)phthalic acid)

IT 58370-80-2 58370-81-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with diaminoaryl derivs.)

IT 58374-11-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with diaminonaphthalene)

IT 58370-83-5 58370-84-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with diaminophenetole)

IT 58370-85-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with naphthalenediamine)

IT 58373-86-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with naphthylenediamine)

IT 58373-87-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with phosphorus oxychloride)

IT 58370-82-4

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sodium phenoxide)

IT 139-02-6

RL: USES (Uses)
(reaction with (chlorosulfonyl)naphthalic anhydride)

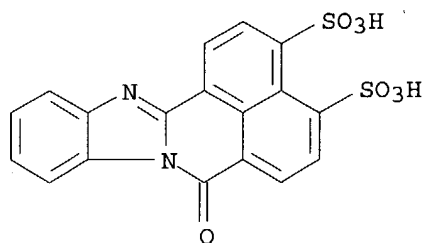
IT 108-95-2, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
(with phthaloperinonesulfonyl chloride)

RN 64193-49-3 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-3,4-disulfonic acid, 7-oxo-,
 disodium salt (9CI) (CA INDEX NAME)
 MF C18 H10 N2 O7 S2 . 2 Na
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
=====	=====	=====	=====	=====	=====
C3N2-C5N-C6- C6-C6	NCNC2-NC5-C6- C6-C6	5-6-6-6-6	C18N2	6841.6.3	1



● 2 Na

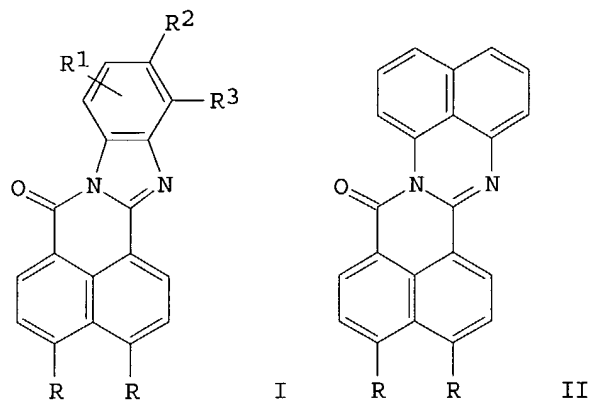
1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 87:153423 CA
 TI Water-soluble dyes for wool
 IN Imahori, Seiichi; Murata, Yukichi; Maeda, Shuichi
 PA Mitsubishi Chemical Industries Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 4 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC C09B057-00
 CC 40-6 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----		-----	-----	-----
PI	JP 52072726	A2	19770617	JP 1975-149840	19751216
	JP 58057463	B4	19831220		
PRAI	JP 1975-149840		19751216		

GI



AB The title dyes I (R = SO₃Na; R₁ = H, Me, OMe, NO₂; R₂, R₃ = H or R₂R₃ = benzo) and II (R = SO₃Na) [64193-50-6] were prepared by reaction of Na₂O₃ with I (R = Cl, Br) and II (R = Cl) [40445-16-7]. For example, I (R = Cl, R₁ = R₂ = R₃ = H) [40445-12-3] was autoclaved with aqueous Na₂SO₃ at 150° for 20 h and salted to give I (R = SO₃Na, R₁ = R₂ = R₃ = H) [64193-49-3], reddish yellow on wool.

ST oxobenzimidazobenzisoquinolinedisulfonate dye wool;
oxobenzisoquinoperimidinedisulfonate dye wool

IT Dyes
(oxobenzimidazobenzisoquinolinedisulfonates and
oxobenzisoquinoperimidinedisulfonates, with high solubility, for wool)

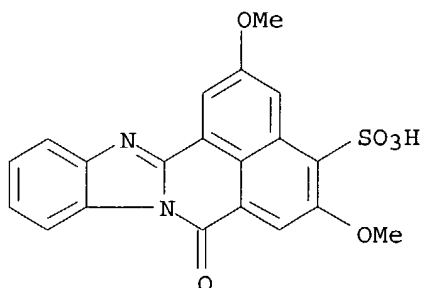
IT 64190-18-7P 64190-19-8P 64190-20-1P 64193-47-1P 64193-49-3P
64193-50-6P
RL: MSC (Miscellaneous); PREP (Preparation)
(dyes, highly soluble, for wool, manufacture of)

IT 40445-12-3 40445-16-7 64190-10-9 64190-21-2 64190-22-3
64193-48-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(sulfonation of)

RN 62599-18-2 REGISTRY
ED Entered STN: 16 Nov 1984
CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-4-sulfonic acid,
2,5-dimethoxymethyl-7-oxo-, sodium salt (9CI) (CA INDEX NAME)
MF C21 H16 N2 O6 S . Na
CI IDS
LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
=====	=====	=====	=====	=====	=====
C3N2-C5N-C6- C6-C6	NCNC2-NC5-C6- C6-C6	5-6-6-6-6	C18N2	6841.6.3	1



D1-Me

● Na

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

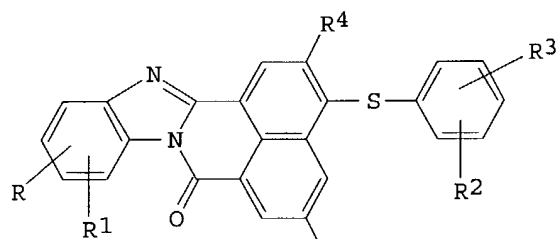
REFERENCE 1

AN 86:191337 CA
TI 1,8-Naphthoylenebenzimidazole derivatives
IN Shirosaki, Tsutomu
PA Nippon Kayaku Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC C09B057-00
CC 40-10 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
Section cross-reference(s): 28

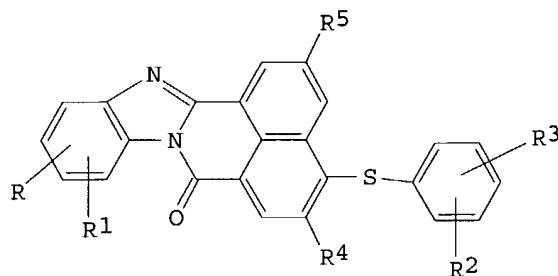
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	-----		-----	-----	-----
PI	JP 51111237	A2	19761001	JP 1975-36069	19750327
PRAI	JP 1975-36069		19750327		

GI



I



II

- AB I-II mixts. (R = H, Me, OMe, Bu, NO₂, Cl, CO₂H; R₁ = H, Me; R₂ = H, NH₂, Bu, Me, OMe; R₃ = H, Cl, Me, CO₂H; R₄ = H, Cl, Br, OH, OMe, OPr; R₅ = H, Cl, Br, OH, OMe, OPr, NO₂, SO₂NMe₂, SO₂NEt₂) useful as thioxanthene dye intermediates and as colorants for plastics and hydrophobic fibers were prepared For example, 1,2-benzenediamine [95-54-5] was stirred with 4-sulfonaphthalic anhydride Na salt [62635-64-7] in water at 98° for 12 h and then autoclaved with 2-aminobenzenethiol [137-07-5] in the presence of K₂CO₃ and Na₂SO₃·7H₂O at 150° for 10 h and at 170° for 12 h to give I-II mixture (all R's = H except R₂ = 2-NH₂); about 34 I-II mixts. were prepared
- ST phenylthionaphthoylenebenzimidazole deriv manuf; naphthoylenebenzimidazole phenylthio deriv
- IT Dyes
(intermediates, (phenylthio)naphthoylenebenzimidazole derivs.)
- IT 41537-57-9P 62602-99-7P
RL: PREP (Preparation)
(manufacture and reaction with aminobenzenethiol)
- IT 62599-17-1P 62599-18-2P 62599-40-0P 62599-41-1P
RL: PREP (Preparation)
(manufacture and reaction with aminomethylbenzenethiol)
- IT 5654-32-0P 5722-97-4P 53304-39-5P 53304-40-8P 62598-76-9P
62598-77-0P 62598-78-1P 62598-79-2P 62598-80-5P 62598-81-6P
62598-82-7P 62598-83-8P 62598-84-9P 62598-85-0P 62598-86-1P
62598-87-2P 62598-88-3P 62598-89-4P 62598-90-7P 62598-91-8P
62598-92-9P 62598-93-0P 62598-94-1P 62598-95-2P 62598-96-3P
62598-97-4P 62598-98-5P 62598-99-6P 62599-00-2P 62599-01-3P
62599-02-4P 62599-03-5P 62599-04-6P 62599-05-7P 62599-06-8P
62599-07-9P 62599-08-0P 62599-09-1P 62599-10-4P 62599-11-5P
62599-12-6P 62599-13-7P 62599-14-8P 62599-15-9P 62599-16-0P
62599-19-3P 62599-20-6P 62599-21-7P 62599-22-8P 62599-23-9P
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62599-29-5P 62599-38-6P 62599-39-7P 62602-96-4P 62602-97-5P
62602-98-6P 62603-00-3P 62603-01-4P 62624-66-2P 62624-67-3P
62624-68-4P 62624-69-5P 62624-70-8P 62635-63-6P 62653-53-6P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)
- IT 62635-64-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzenediamine)
- IT 95-54-5, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sulfonaphthalic anhydride sodium salt)

IT 106-45-6 137-07-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sulfonaphthoylenebenzimidazole)

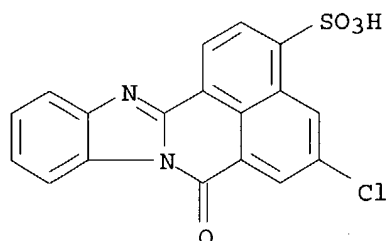
IT 2396-68-1 23451-96-9

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sulfonaphthoylenebenzimidazole derivs.)

RN 62599-40-0 REGISTRY
 ED Entered STN: 16 Nov 1984
 CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-3-sulfonic acid,
 5-chloromethyl-7-oxo-, sodium salt (9CI) (CA INDEX NAME)
 MF C19 H11 Cl N2 O4 S . Na
 CI IDS
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
=====	=====	=====	=====	=====	=====
C3N2-C5N-C6- C6-C6	NCNC2-NC5-C6- C6-C6	5-6-6-6-6	C18N2	6841.6.3	1



D1-Me

● Na

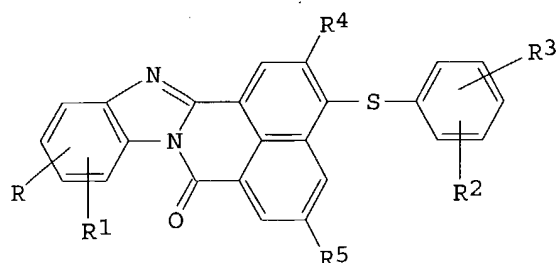
1 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

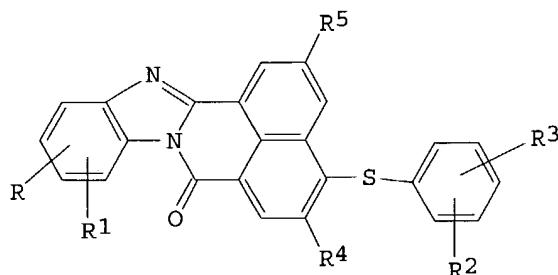
AN 86:191337 CA
 TI 1,8-Naphthoylenebenzimidazole derivatives
 IN Shirotsaki, Tsutomu
 PA Nippon Kayaku Co., Ltd., Japan
 SO Jpn. Kokai Tokkyo Koho, 6 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC C09B057-00
 CC 40-10 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
 Section cross-reference(s): 28
 FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI JP 51111237	A2	19761001	JP 1975-36069	19750327
PRAI JP 1975-36069		19750327		

GI



I



II

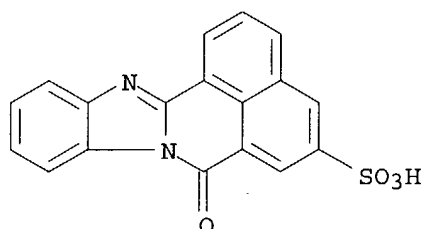
- AB I-II mixts. (R = H, Me, OMe, Bu, NO₂, Cl, CO₂H; R₁ = H, Me; R₂ = H, NH₂, Bu, Me, OMe; R₃ = H, Cl, Me, CO₂H; R₄ = H, Cl, Br, OH, OMe, OPr; R₅ = H, Cl, Br, OH, OMe, OPr, NO₂, SO₂NMe₂, SO₂NEt₂) useful as thioxanthene dye intermediates and as colorants for plastics and hydrophobic fibers were prepared For example, 1,2-benzenediamine [95-54-5] was stirred with 4-sulfonaphthalic anhydride Na salt [62635-64-7] in water at 98° for 12 h and then autoclaved with 2-aminobenzenethiol [137-07-5] in the presence of K₂CO₃ and Na₂SO₃·7H₂O at 150° for 10 h and at 170° for 12 h to give I-II mixture (all R's = H except R₂ = 2-NH₂); about 34 I-II mixts. were prepared
- ST phenylthionaphthoylenebenzimidazole deriv manuf; naphthoylenebenzimidazole phenylthio deriv
- IT Dyes
(intermediates, (phenylthio)naphthoylenebenzimidazole derivs.)
- IT 41537-57-9P 62602-99-7P
RL: PREP (Preparation)
(manufacture and reaction with aminobenzenethiol)
- IT 62599-17-1P 62599-18-2P 62599-40-0P 62599-41-1P
RL: PREP (Preparation)
(manufacture and reaction with aminomethylbenzenethiol)
- IT 5654-32-0P 5722-97-4P 53304-39-5P 53304-40-8P 62598-76-9P
62598-77-0P 62598-78-1P 62598-79-2P 62598-80-5P 62598-81-6P
62598-82-7P 62598-83-8P 62598-84-9P 62598-85-0P 62598-86-1P
62598-87-2P 62598-88-3P 62598-89-4P 62598-90-7P 62598-91-8P
62598-92-9P 62598-93-0P 62598-94-1P 62598-95-2P 62598-96-3P
62598-97-4P 62598-98-5P 62598-99-6P 62599-00-2P 62599-01-3P
62599-02-4P 62599-03-5P 62599-04-6P 62599-05-7P 62599-06-8P
62599-07-9P 62599-08-0P 62599-09-1P 62599-10-4P 62599-11-5P
62599-12-6P 62599-13-7P 62599-14-8P 62599-15-9P 62599-16-0P
62599-19-3P 62599-20-6P 62599-21-7P 62599-22-8P 62599-23-9P
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62599-29-5P 62599-38-6P 62599-39-7P 62602-96-4P 62602-97-5P
62602-98-6P 62603-00-3P 62603-01-4P 62624-66-2P 62624-67-3P
62624-68-4P 62624-69-5P 62624-70-8P 62635-63-6P 62653-53-6P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)
- IT 62635-64-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with benzenediamine)
- IT 95-54-5, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with sulfonaphthalic anhydride sodium salt)
IT 106-45-6 137-07-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sulfonaphthoylenebenzimidazole)
IT 2396-68-1 23451-96-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with sulfonaphthoylenebenzimidazole derivs.)

RN 521307-85-7 REGISTRY
 ED Entered STN: 28 May 2003
 CN 7H-Benzimidazo[2,1-a]benz[de]isoquinoline-5-sulfonic acid, 7-oxo- (9CI)
 (CA INDEX NAME)
 FS 3D CONCORD
 MF C18 H10 N2 O4 S
 SR CA
 LC STN Files: CA, CAPLUS

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
=====	=====	=====	=====	=====	=====
C3N2-C5N-C6- C6-C6	NCNC2-NC5-C6- C6-C6	5-6-6-6-6	C18N2	6841.6.3	1



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
=====	=====	=====	=====
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	1	pH 7	(1) ACD
Bioconc. Factor (BCF)	1	pH 8	(1) ACD
Bioconc. Factor (BCF)	1	pH 10	(1) ACD
Freely Rotatable Bonds (FRB)	2		(1) ACD
H acceptors (HAC)	6		(1) ACD
H donors (HD)	1		(1) ACD
Koc (KOC)	5.50	pH 1	(1) ACD
Koc (KOC)	2.88	pH 4	(1) ACD
Koc (KOC)	1	pH 7	(1) ACD
Koc (KOC)	1	pH 8	(1) ACD
Koc (KOC)	1	pH 10	(1) ACD
logD (LOGD)	0.93	pH 1	(1) ACD
logD (LOGD)	0.65	pH 4	(1) ACD
logD (LOGD)	-0.65	pH 7	(1) ACD
logD (LOGD)	-0.67	pH 8	(1) ACD
logD (LOGD)	-0.67	pH 10	(1) ACD
logP (LOGP)	3.430+/-0.620		(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	350.35		(1) ACD
pKa (PKA)	4.00+/-0.20	Most Basic	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
Solaris V4.76 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 138:370267 CA
TI Soluble polycyclic dyes
AU Wolska, Anna; Wojciechowski, Krzysztof; Niewiadomski, Zbigniew
CS Inst. Barwnikow i Produktow Org., Zgierz, 95-100, Pol.
SO Barwniki, Srodki Pomocnicze (2002), 46(1/2), 15-26
CODEN: BSPOEM; ISSN: 0867-7824
PB Instytut Barwnikow i Produktow Organicznych
DT Journal
LA Polish
CC 41-5 (Dyes, Organic Pigments, Fluorescent Brighteners, and Photographic Sensitizers)
Section cross-reference(s): 40, 28
AB The article describes the preparation of soluble polycyclic dyes containing imide or imidazole moieties and the possibility to using them for dyeing cellulosic fibers as direct dyes. The dyes were obtained by condensation of 1,8-naphthalenedicarboxylic acid, 1,4,5,8-naphthalenetetracarboxylic acid, or 3,4,9,10-perylenetetracarboxylic acid with aniline or o-phenylenediamine, followed by sulfonation of the condensation products. Depending on the dye type, cotton fabric was dyed to attain yellow, blue, or orange color. The importance of sulfonation conditions in obtaining dyes with good vat dyeing properties is discussed.
ST polycyclic vat dye prepn cotton fabric dyeing; sulfonated imide imidazole group contg polycyclic vat dye prepn
IT Textiles
(cotton; preparation of polycyclic vat dyes and their use in cotton fabric dyeing)
IT Sulfonation
(effect of sulfonation conditions on preparation of polycyclic vat dyes and use of the obtained dyes in cotton fabric dyeing)
IT Vat dyeing
(preparation of polycyclic vat dyes and their use in cotton fabric dyeing)
IT Dyes
(vat; preparation of polycyclic vat dyes and their use in cotton fabric dyeing)
IT 440093-45-8P 440093-46-9P 521307-84-6P 521307-85-7P 521307-86-8P
521963-64-4P 521963-65-5P
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); PROC (Process); USES (Uses)
(dye; preparation of polycyclic vat dyes and their use in cotton fabric dyeing)
IT 128-65-4P 4216-02-8P 4424-06-0P 23749-58-8P 55034-79-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate in dye preparation; preparation of polycyclic vat dyes and their use in cotton fabric dyeing)
IT 62-53-3, Aniline, reactions 81-30-1 85-44-9, Phthalic anhydride
95-54-5, o-Phenylenediamine, reactions 128-69-8 6914-98-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant in dye preparation; preparation of polycyclic vat dyes and their use in

cotton fabric dyeing)